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Hybrid Multiscale Method for Coupling Atomistic and Continuum Models

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In this project [3] we develop and test a hybrid multiscale method for coupling atomistic and continuum models. We perform Monte Carlo (MC) simulation for random walk in microscale domains and solve the diffusion equation on the macroscale. The numerical results depend strongly on the efficient and stable coupling between the microscale and macroscale solvers. The present work gives the principles of the technique and shows the potential for future practical applications, e.g. interface tracking for epitaxial growth of thin films and complex fluids.

Multiscale modeling that couple atomistic and continuum simulations has recently become one of the most active research areas in applied science. With rapidly growing computing power, we are more capable of modeling the details of physical process. Meanwhile, several multiscale methods have been proposed to design efficient numerical methods for bridging the differences between long and short time or space scales, such as heterogeneous multiscale method (HMM) introduced by E and Engquist [1] and patch dynamics designed by Kevrekidis, Gear and etc [4][2]. When successfully applied, these methods can use microscopic descriptions of a problem to create a system-level framework that helps predict macroscopic properties from direct numerical simulations of relevant microscopic models.

The basic setup in present project is following. Suppose we have a set of variables $U(x,t)$ to describe the macroscale process at time t. To compute the macroscopic variables at the next time step $t+\Delta t$, we extract the data needed in the macroscale solver, for example the particle flux, from the microscopic model. In order for the microscale states u to be consistent with the local macroscale states U, certain constraints are imposed in the microscopic model, usually through the imposition of some boundary conditions. The microscopic data are then processed using statistical averaging to provide the needed macroscale data. These data are finally feeded back to the macroscale solver and $U(x,t+\Delta t)$ are calculated.

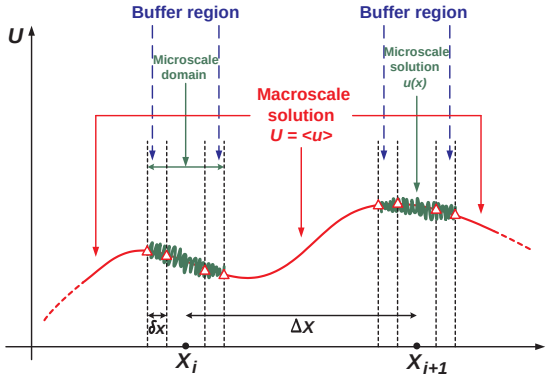

Figure 1. One-dimensional physical system [2]. The microscale variable $u(x)$ varies rapidly, but the macroscopic-averaged variables $U = (\langle u\rangle, \langle u_x\rangle, \langle u_{xx}\rangle$ and so on) vary slowly. The boundary conditions for the microscale solvers are defined in the buffer regions surrounding each microscale domains. The communication between the macroscale and microscale models is performed in the buffer regions.

The key to the feasibility and efficiency of such an approach is the possibility that the microscale model does not need to be solved over the whole computational domain, but rather over a small region near the interface where data estimation is carried out; see Figure 1. Furthermore, the separation of the macroscopic and microscopic scales of the system is also an advantage of this approach.

Algorithm

Step 0: Set up the microscale grids with length scale δx and the macroscale grids with length scale Δx. Both microscale and macroscale initial data are defined at grid points.

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Step 1: Define the buffer region which covers several microscale grid sizes in one macroscale cell at the interface between the two different scales. The information transformation from the macroscale to the microscale models will be performed here.

Step 2: Advance the macroscale model for one macroscale time step Δt to obtain solution U^n. Standard finite difference or finite volume method can be used to solve the diffusion equation.

Step 3: With macroscopic solution U^{n-1} and U^n, reconstruct the microscale initial and boundary conditions for each MC simulation to match the average macroscale quantities in the buffer region. The interpolation in both time and space for macroscale states are needed. The microscale boundary conditions agree statistically with the macroscale interpolant. Here the macroscale provides information for the microscale.

Step 5: Advance the microscale model via MC simulation for one macro-step Δt, which takes many small micro-steps δt.

Step 6: In the microscale region close to the interface, we compute the particle flux F^n or the local average of the microscale solution $u(x)$ to define the macroscale interface/boundary conditions for the macroscopic model. This is the step where the microscale supplies information to the macroscale.

Step 7: Stop if the desired time is reached in the macroscopic model. Otherwise, repeat from Step 2 using the new flux F^n to replace the finite difference or using the local average as the Dirichlet boundary condition in the finite difference scheme to advance the macroscopic solution to time t^{n+1}. □

In Figure 2, agreement between the hybrid results and the true solution is excellent at all time in both cases (b) and (d), which indicates the efficacy of the coupling atomistic and continuum simulations.

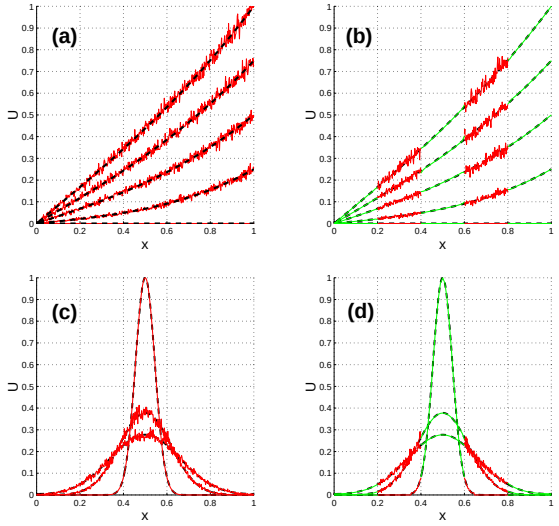

Figure 2. Results at different times. In each panel the true solutions are dashed curves. In (a) and (b), we show the growth of an initial zero concentration profile. In (c) and (d), we show the decay of an initial Gaussian concentration profile. In (a) and (c), we perform the full MC simulation with $\delta x = 0.002$. In (b) and (d), we solve hybrid models with macroscale grid size $\Delta x = 0.01$ and microscale grid size $\delta x = 0.002$; MC is performed on regions $(0.2, 0.4)$ and $(0.6, 0.8)$ and the diffusion equation is solved on other regions.

Acknowledgements

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